

A Simple General Scripting Prototype in Matlab

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Disclaimer : no nice images, looks like a boring talk ?

Data Analysis: 10 years maturing

Minimize coding:

stick to simple and accurate operations.

GUI takes too much time. Will be built on top afterwards.

Lower maintenance:

Project size should not exceed a few Mb code

Easy install (else users give-up):

Minimize dependencies. Embed dependencies ?

Adaptable to any problem:

Initial infrastructure must be general (no n, X, \dots).

Focus on LOAD, MATH, FIT, SAVE and simple PLOT.

Load

General import method

load(file) should work, for all → automatic file analysis

General tool for text based files <<http://looktxt.sourceforge.net>>

Dedicated wrappers for binary files (incl. NeXus)

File imported as a **structure**, whatever be the initial format

Definition of signal, axes, *etc*, is dynamic

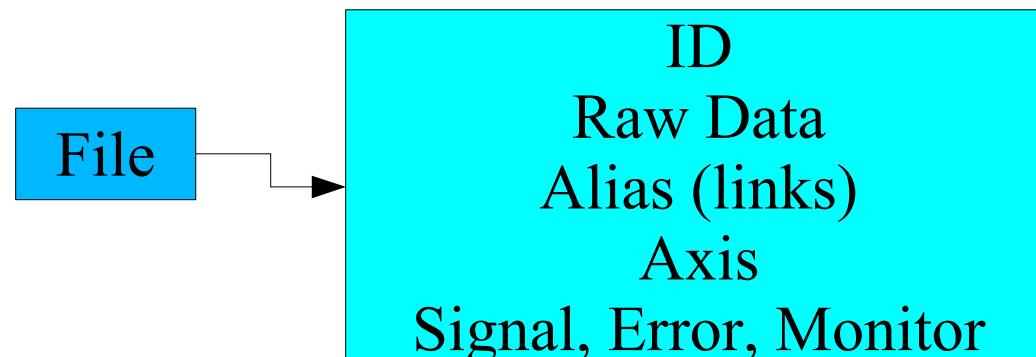
An Alias is a **link** to an other field in the structure (link)

Signal and axes are assigned to Aliases or some data or expression

An **operation** applies on Signal and axes

Data can be modified **dynamically**

Handles any data set **dimensionality**



Math: unitary operators

Apply on Signal and Error bars

- ★ Negation
- ★ Logical negation (not)
- ★ Casting to other types
- ★ Transposition
- ★ Rounding
- ★ Unary Tests (is something)
- ★ Acos, asin, atan cos, exp, log, log10, sin, sqrt, tan, abs
- ★ Peak finding
- ★ Integration, sum, projection, gradient

Math: binary operators

Apply on Signal, Error bars and Monitor, upon axis intersection

Re-sample transparently axes and signal when dimensions match

Extend transparently axes and signal when dimensions do not match

★+ - / *

★Combine (merge)

★Power

★Comparisons ($>$ $<$ \leq and or ...)

★Interpolation

★Re-sampling and axis changes (apply gradient)

★Catenate and dimensionality extension

Enable in principle *any* data analysis.

Fit and Optimization

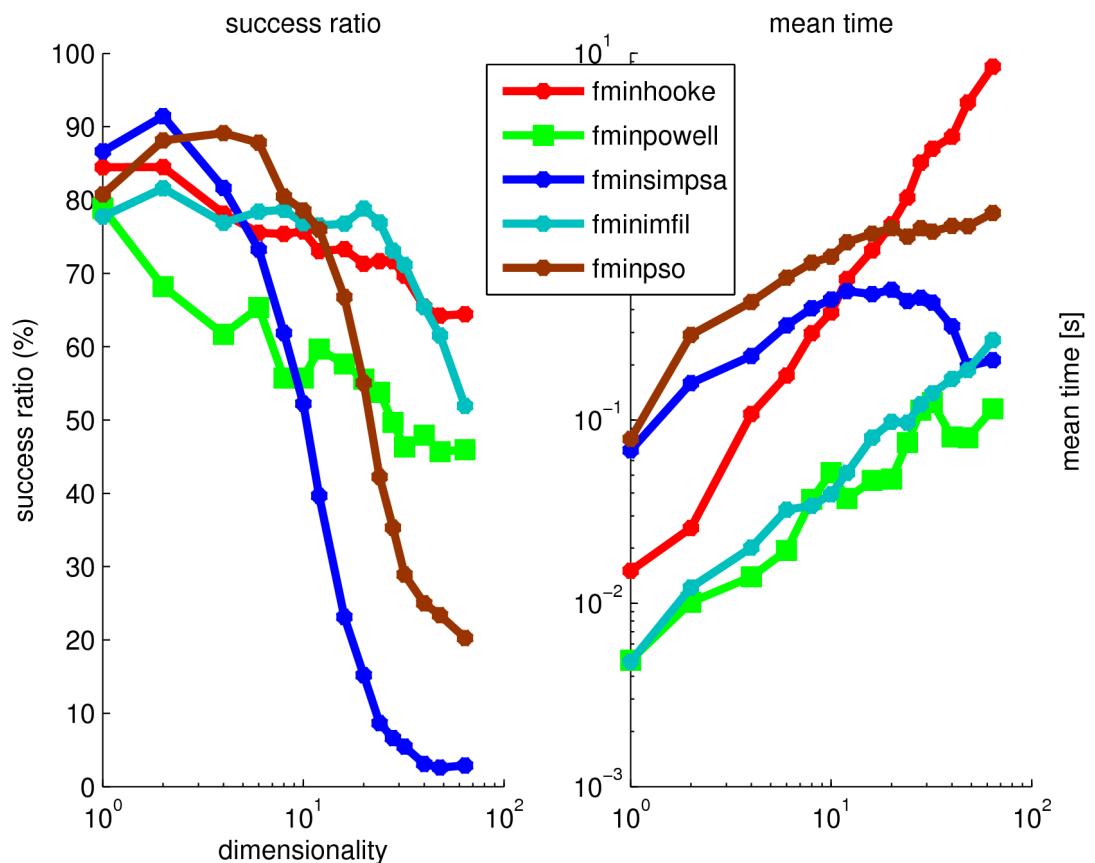
General fitting method

Find optimal parameters for a model to match a data set.

Optimizer calls are standardized, obtained from e.g. *Matlab Central*

Powell Search	(by Secchi)	[fminpowell]
Shor r-algorithm	(by Kuntsevich)	[fminralg]
Evolution Strategy with Covariance Matrix Adaptation	(CMA-ES by Hansen)	[fmincmaes]
Nelder-Mead Simplex	(by Kelley)	[fminsimplex]
Steihaug Newton-CG-Trust	(by Kelley)	[fminnewton]
Random Gradient	(by Belur)	[fmingradrand]
Unconstrained Implicit filtering	(by Kelley)	[fminimfil]
Broyden-Fletcher-Goldfarb-Shanno	(by Kelley)	[fminbfgs]
Hooke-Jeeves direct search	(by Kelley)	[fminhooke]
Simulated Annealing	(by Vandekerckhove)	[fminanneal]
simplex/simulated annealing	(by Donckels)	[fminsimpsa]
Shuffled Complex Evolution	(by Donckels)	[fminsce]
Particle Swarm Optimization	(by Donckels)	[fminpso]
Genetic Algorithm	(real coding by Ivakpour)	[fminga]
unscented Kalman filter optimizer	(by Cao)	[fminkalman]
Nelder-Mead simplex	(by Salvado/Matlab)	[fminsearchOS]
Standard Simplex-based Matlab optimizer	(by Matlab)	[fminsearch]
Particule Swarm Optimizer	(by Leontitsis)	[fminswarm]
Hybrid Particule Swarm Optimizer	(by Leontitsis)	[fminswarmhybr]
Adaptive Random Search	(by Secchi)	[fminrand]
Multidirectional search	(by Kelley)	[fminmulti]

Best Optimizers



23 optimizers
52 test problems
Up to dim=64
MC procedure

Dim <=3
Dim <=5
Best general method

simplex/simulated annealing
particle swarm optimizer
Unconstrained Implicit filtering

General export method

Support text formats

Support bitmap and vectorial images

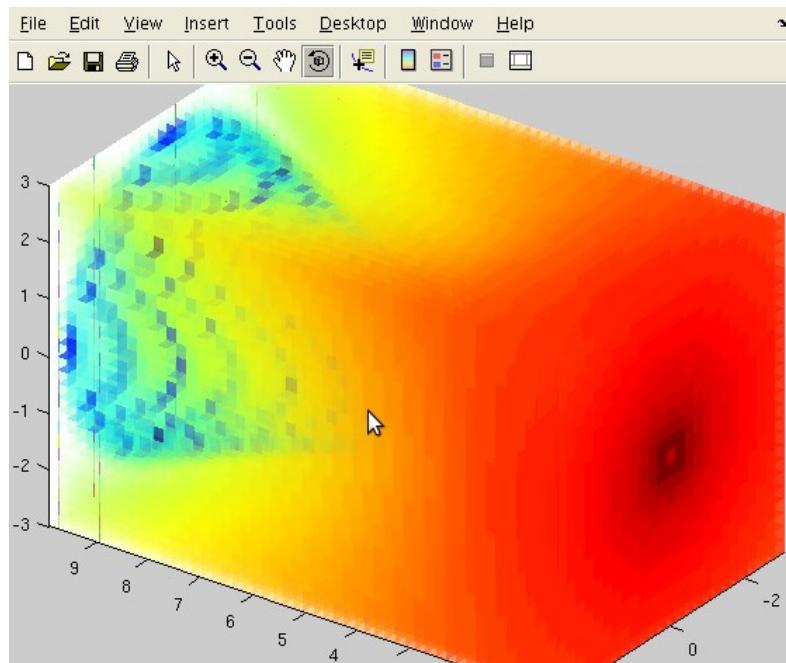
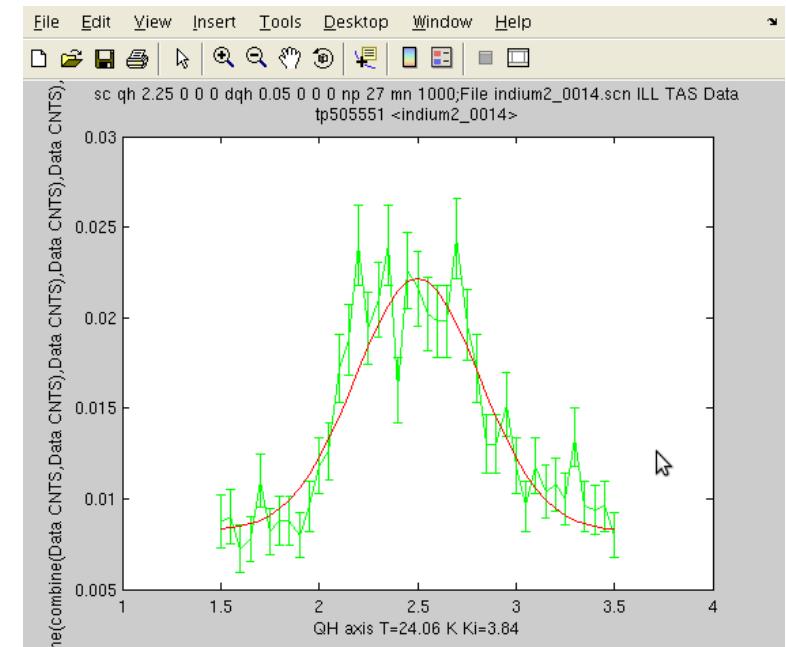
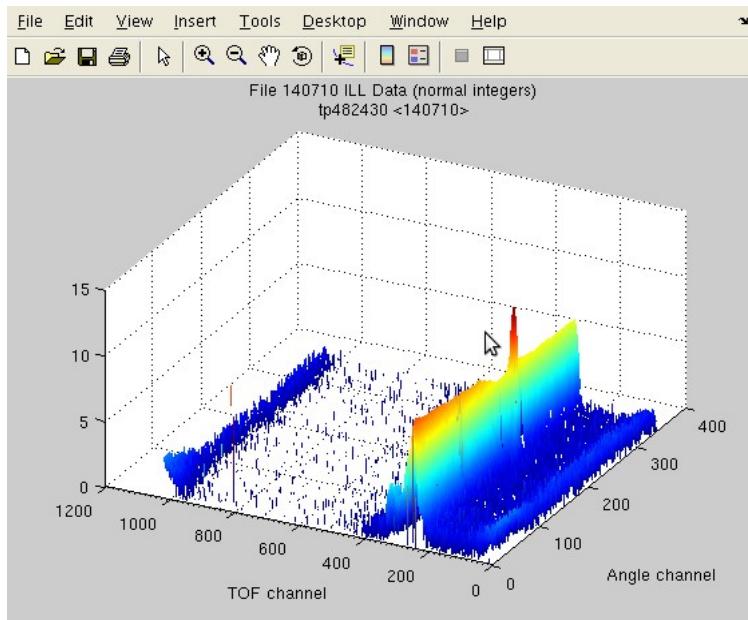
Support *Nexus*

Plotting (basic)

Simple plotting

1D, 2D and 3D plots

UI interaction through contextual menu



Prototype coding

Matlab based for fast production – Octave compatible

Package architecture:

- @iData: main object definition and methods
- iFiles: read files and return structures
- iOptim and iFuncs: fitting/optimization routines

Download prototype

<<http://cvs.mccode.org/cgi-bin/viewvc.cgi/?root=iFitCVS>>

Or ask me <farhi@ill.eu>

No GUI yet, because it uses too much time.

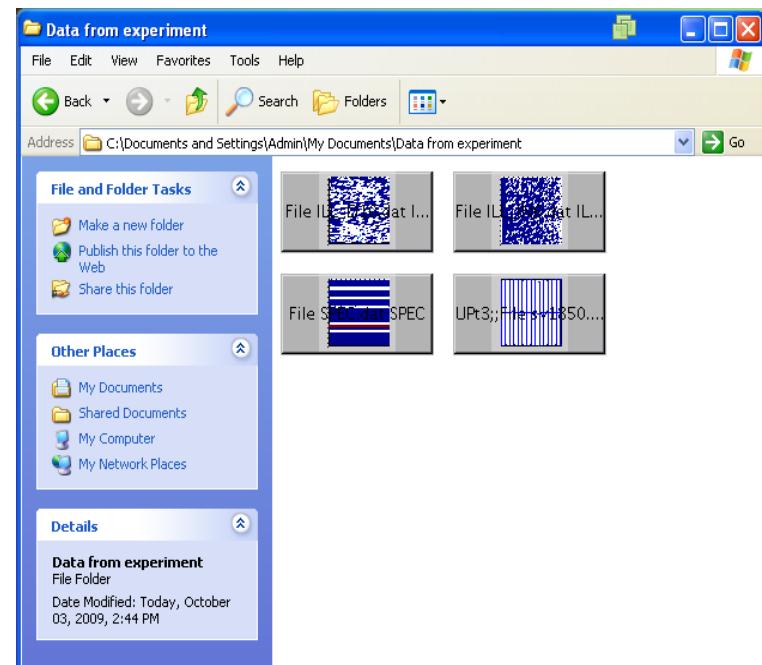
Interface (GUI)

Passive GUI: use existing File Managers

- Generate thumbnails from data files (Text based/HDF).
- Allows to display as icons/lists and quickly sort/browse many files.
- Fully integrated into operating systems.
- Propose dedicated actions in contextual menus.
- Provide basic data viewer.

Dedicated GUI:

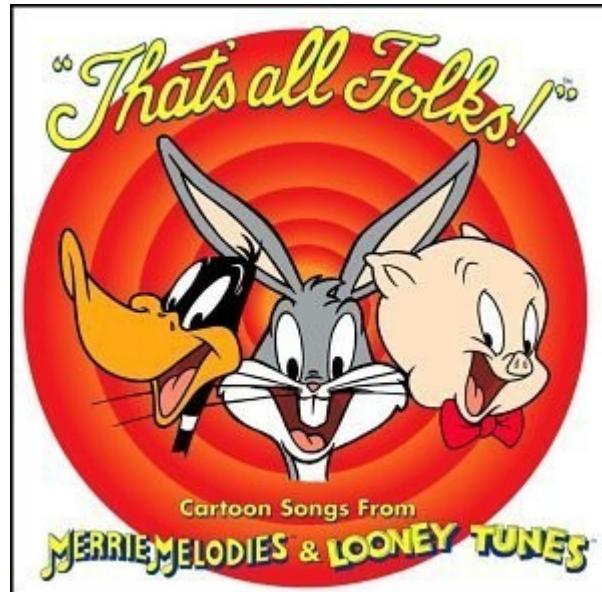
- Should inspire from File Managers
- And MovieMaker/iPhoto/iMovie
- Trigger scripts
- Provide basic Math
- Provide Load/Save
- Provide Plotting
- Provide Fitting



Must **not be too ambitious**, so that deliverables can be produced fast.

Time for a demo

- Load
- Object structure
- Plot
- Math
- Fit



Just for fun : find the BUG ?

Simulate:

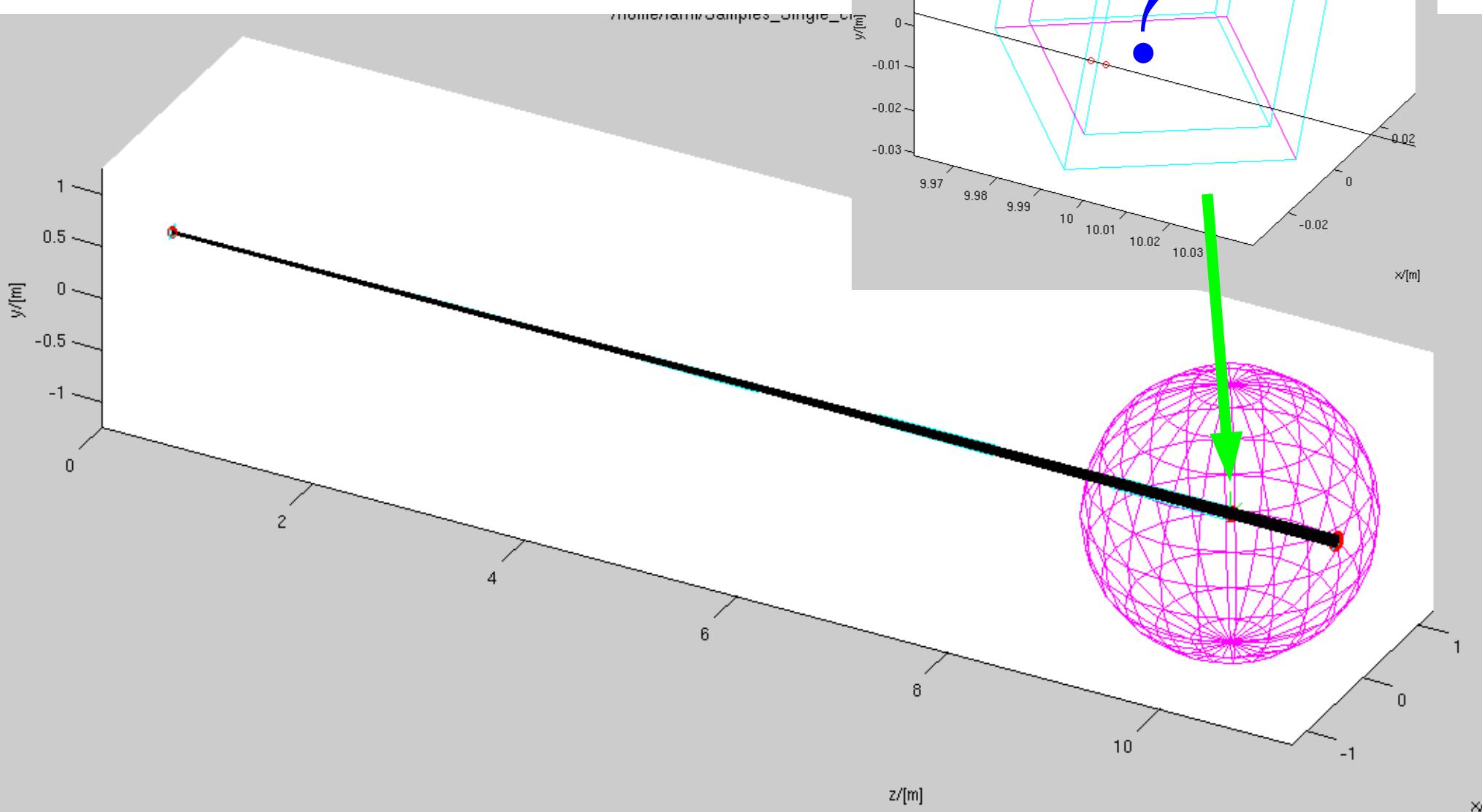
- A neutron source with varying wavelength λ
- A box made of aluminium
- A secret item in the box (the BUG)
- A large scattering detector
- A transmission detector

We use:

- McStas
- OFF geometry in PowderN and Single_crystal components
- Matlab iData prototype for 3D rendering

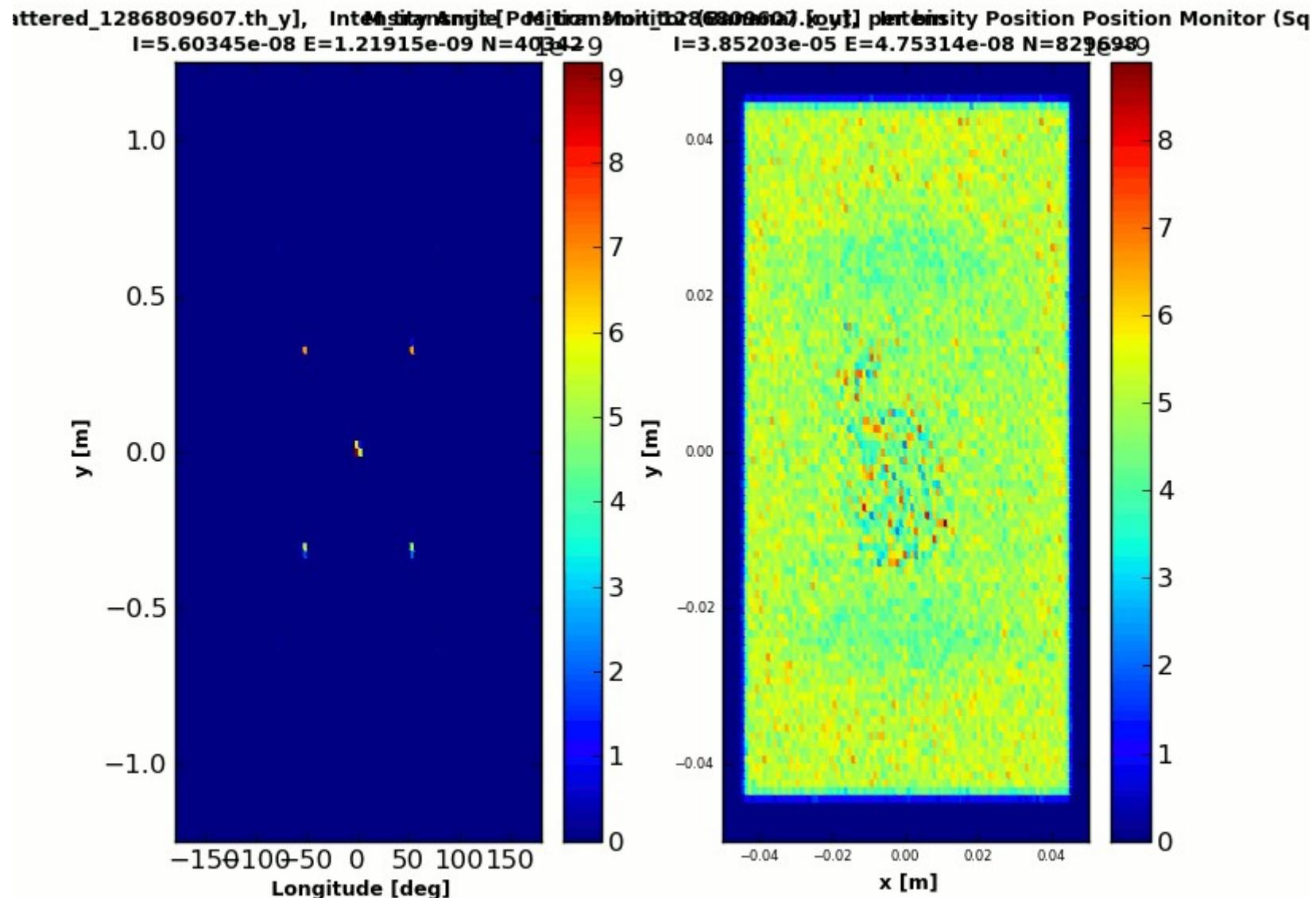
Model geometry

Scan wavelength from $\lambda=1$ to 3 Å



Import and plot results

Using McStas/McPlot



Import and plot results

Using Matlab/iData

```
s=iData({ '0/M_scatt*', '1/M_scatt*', ... }) ;
S3=cat(3,s) ;
plot(S3) ;    % scattered signal

t=iData({ '0/M_trans*', '1/M_trans*', ... }) ;
T3=iData(3,t) ;
plot(T3) ;    % transmitted signal
```

